Torsion 73 [!#1;r{5-8}:1]@[NX2;r{5-8}:2]@;-[S;r{5-8}:3]@[!#1;r{5-8}:4] **Binned Counts** 0.06 Gaussian Fit **ETKDG Fit** 0.05 Probability per 10° Bin 0.04 0.03 -0.02 0.01 0.00 60 120 180 Torsion (°)